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### A developmental research on introducing the quantum mechanics formalism at university level

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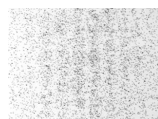
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## Appendix A

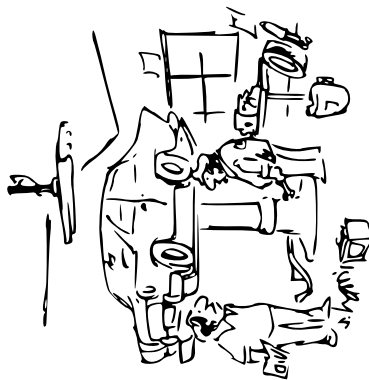
# Designed Study Material

The study material used in the last research round in the Quantum Chemistry course is reproduced verbatim on the following pages. Short answers to the questions are provided. A booklet without these answers was handed out to the students. The text is translated from Dutch.



Quantum Chemistry 2008-2009  
 assignments for the studio course meetings  
 with answers

Lodewijk Koopman  
 January 29, 2009



“Actually I started out in quantum mechanics, but somewhere along the way I took a wrong turn.”

Cover illustration: S. Harris, <http://www.sciencecartoonsplus.com/>.

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## Introduction

In the first four meetings of the Quantum Chemistry course we will give an introduction to quantum theory. We will try to reach this theory in a few steps. This will take about two weeks, which of course is very fast. Quantum theory itself was developed roughly between 1900 (Max Planck) and 1926 (Erwin Schrödinger), and since then the development has not stopped. This history will not be repeated. We do want to have a look at some arguments that have led to quantum theory. This will be done by first considering experiments that cannot be explained by classical physics.

The assignments in this booklet are probably different from what you are used to. The questions are often open ended and multiple answers might be 'correct'. It is therefore important to discuss the answers with each other. Be sure to ask for assistance in time if you think you are stuck, or when you do not understand the question! The first four meetings will be given in the form of a studio course. This combines lecture and problem solving session.

If you see the following symbol in the margin:  $\oplus$ , go to the Blackboard site and make the corresponding assignment to refresh your prior knowledge on the current topic.

Good luck, and have fun with the assignments.

## Studio course 1: Matter waves

### 1.1 Double slit experiment

It is sometimes said that electrons interfere. Interference is a phenomenon associated with waves, not with particles. In the next few assignments we carefully explore what the basis is to speak of interference when talking about electrons and to what extent we can compare this with classical waves. In order to do so, we first have a closer look at interfering water waves in a double slit experiment and use our insights to understand experiments for light and electrons that are analogous to that of the double slit experiment for water. The experimental setup of these experiments is schematically shown in Figure 1. The pattern that is visible for water, light, and electrons is shown in Figures 2, 3, and 4 respectively.

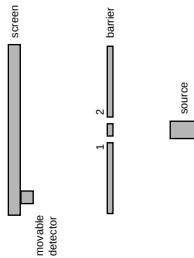


Figure 1: Schematic representation of setup of all double slit experiments in this assignment (top view). The slits are numbered 1 and 2.

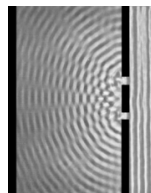


Figure 2: Water: pattern behind double slit (top view).

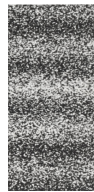


Figure 3: Light: pattern on the screen behind double slit.

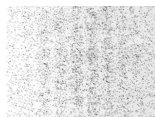


Figure 4: Electrons: pattern on the screen behind double slit.

1.1.1 Water

We are going to mathematically describe/explain the pattern that is visible behind the two slits in Figure 2. First have a look at the situation when one of the slits is closed. The waves that emerge are then (approximately) circular (see the figure on the right). The displacement of such a wave on a distance  $r$  from the slit, at time  $t$  is given by:



$$u(r, t) = u_0 \cos(kr - \omega t), \quad (1)$$

⊕ where  $k = 2\pi/\lambda$  is the wave number, with the wave length  $\lambda$ , the angular frequency  $\omega = 2\pi f$ , and the frequency  $f$ . In reality the amplitude  $u_0$  also depends on  $r$ , but we will ignore that for now.

1. Explain that  $u(r, t)$  describes a circular wave. Show for instance that at a fixed time  $t$  points with maximum displacements all lie on a circle.

**Answer** If we set the time equal to  $t = 0$ , then the displacement is maximal (positive) when  $kr = 2n\pi$ , with  $n = 1, 2, 3, \dots$ , so then  $r = 2n\pi/k$ . This corresponds to points lying on a circle. Stated differently: for fixed  $r$  (points on a circle with radius  $r$ ), the displacement is constant.

2. In what direction is the wave moving?

**Hint** Sketch a graph of the wave as a function of  $r$ , where you set the time to  $t = 0$ . Make another sketch of the wave, a little time later; for instance  $t = \pi/2\omega$ .

**Answer** The wave moves 'outward' (increasing  $r$ ). If we look at the cosine for a fixed argument (fixed displacement), then for increasing time,  $r$  has to increase to keep the argument constant. This also becomes visible when the graphs suggested by the hint are drawn (not reproduced here). For small steps  $\Delta t$  we see the graph of  $u(r, t)$  moving to the right, which corresponds to 'outward', since  $r$  is the radius.

⊕ The calculations that follow are more straightforward when we write the wave  $u(r, t)$  as a complex exponential:  $e^{ix} = \cos x + i \sin x$ . In our case we write:

$$\begin{aligned} \hat{u}(r, t) &= u_0 e^{i(kr - \omega t)}, \\ u(r, t) &= \operatorname{Re} \hat{u}(r, t). \end{aligned}$$

To check whether the the circular waves, described by the function  $\hat{u}(r, t)$ , can explain the interference pattern, we calculate what the pattern looks like based on such waves and compare this with the pattern that is observed. The wave emerging from slit 1 when slit 2 is closed is called  $\hat{u}_1$ , and vice versa. The displacement of the wave when both slits are opened is called  $\hat{u}_{\text{pattern}}$ .

3. How does  $\hat{u}_{\text{pattern}}$  depend on  $\hat{u}_1$  and  $\hat{u}_2$ ?

**Answer** The effect of two slits opened, compared to one slit opened is that the displacement of the individual waves add up:  $\hat{u}_{\text{pattern}} = \hat{u}_1 + \hat{u}_2$ .

The pattern in Figure 2, and thus  $\hat{u}_{\text{pattern}}$ , is two dimensional. This is difficult to plot in a graph. It would be more useful to calculate the displacement along a screen placed at a distance  $L$  from the double slit (see Figure 1).

4. Try to find an expression for  $\hat{u}_{\text{pattern}}$  at a distance  $L$  from the double slit as a function of the location  $x$  along the screen. Use the coordinates shown in Figure 5 and 6. Because we assume that  $\alpha$  is small, you may use  $\tan \alpha \approx \sin \alpha$ .

**Hint** The two waves are circular relative to different points. What will change in the general expression for a wave, Equation (1)?

**Answer** We calculate the displacement at a distance  $L$  from the double slit along a line parallel to the double slit. We use that  $\hat{u}_{\text{pattern}} = \hat{u}_1 + \hat{u}_2$  (prior answer) and:  $\hat{u}_1 = \hat{u}_1(r_1, t)$ ,  $\hat{u}_2 = \hat{u}_2(r_2, t)$ . The derivation is as follows:

Assuming that two circular waves emerge from the slits, the two waves (monochromatic and in phase) can be described by:

$$\begin{aligned} \hat{u}_1(r_1, t) &= u_0 e^{i(kr_1 - \omega t)}, \\ \hat{u}_2(r_2, t) &= u_0 e^{i(kr_2 - \omega t)}. \end{aligned}$$

For circular waves (actually cylindrical waves) the amplitude falls off as  $1/r$ , but we ignore that here. The real waves are given by  $\operatorname{Re} \hat{u}_{1,2}$ , with amplitude  $|\hat{u}_{1,2}|$ . At a distance  $L$  from the double slit, we observe the sum of these two waves:

$$\begin{aligned} \hat{u}(x, t) &= \hat{u}_1(r_1, t; y = L) + \hat{u}_2(r_2, t; y = L), \\ &= u_0 e^{i(kr_1 - \omega t)} + u_0 e^{i(kr_2 - \omega t)}, \\ &= u_0 e^{-i\omega t} \left( e^{ikr_1} + e^{ikr_2} \right). \end{aligned}$$

The distances  $r_1$  and  $r_2$  can be expressed in terms of the slit separation  $d$ , the distance to the screen  $L$ , and the location along the screen  $x$ .

We assume that the slit separation is small compared to the screen distance:  $d/L \ll 1$ . The lines from the slits to a point  $P$  on the screen are then approximately parallel. We consider points close to the axis of symmetry, such that  $\alpha \approx 0$ . We then find:

$$\begin{aligned} r_1 &= r + \frac{1}{2} \Delta r, \\ r_2 &= r - \frac{1}{2} \Delta r, \\ \Delta r &= d \sin \alpha, \\ &\approx \frac{xd}{L}, \\ r &= \sqrt{x^2 + L^2}. \end{aligned}$$

Using this result in the expression for  $\hat{u}(x,t)$  gives:

$$\begin{aligned}\hat{u}(x,t) &= u_0 \exp(i(k\sqrt{x^2 + L^2} - \omega t)) \left[ \exp(i\frac{kd}{2L}x) + \exp(-i\frac{kd}{2L}x) \right], \\ &= 2u_0 \exp(i(k\sqrt{x^2 + L^2} - \omega t)) \cos\frac{kd}{2L}x.\end{aligned}$$

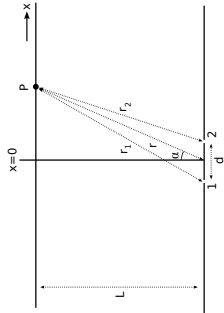


Figure 5: Schematic representation of the double slit.

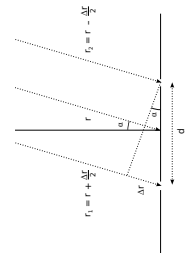


Figure 6: Detail of the double slit setup.

If we plot the real part of  $\hat{u}_{\text{pattern}}$  for different moments in time in sequence, the result is an animation. View the animation on Blackboard: **Assignments** → **Studio Course 1**.

5. Compare the animation to the function  $\hat{u}_{\text{pattern}}$  and explain what you see. Where does constructive interference occur? Where does destructive interference occur? What part of the function  $\hat{u}_{\text{pattern}}$  describes this?

**Answer** For a fixed  $x$ , the complex exponential will only cause the complex vector to rotate in time. The maximum displacement of this factor equals 1. The cosine is independent of time; this describes the static image of the interference pattern. For certain fixed values of  $x$  there is destructive interference, for other values constructive interference. The interference pattern is thus characterized by a maximum displacement (amplitude) of the combined waves.

6. Next compare the animation to the pattern in Figure 2. In what way do the two correspond to each other?

**Answer** The animation is like a cross-section along the screen of the pattern visible in Figure 2. The locations on the screen where the water does not oscillate correspond to certain places in the animation where no oscillation is visible as well. In between the water oscillates heavily.

7. The waves move up and down in time. The **maximum displacement** is called the **amplitude**. Show that the amplitude as function of the location  $x$  is given by:

$$A(x) = 2u_0 \left| \cos\left(\frac{kd}{2L}x\right) \right|. \quad (2)$$

**Hint** Show that the amplitude of a complex wave  $\hat{u}$  is equal to the amplitude of the real wave and that you can write this as  $|\hat{u}| \equiv \sqrt{\hat{u}^* \hat{u}}$ , with  $\hat{u}^*$  the complex conjugate of  $\hat{u}$ . (Also refer to the syllabus of Calculus.)

**Answer** Use the hint:  $|\hat{u}| = \sqrt{\hat{u}^* \hat{u}}$ . The complex exponential is only a phase factor and drops out, so for a fixed  $x$ , the maximum displacement is:

$$2u_0 \left| \cos\left(\frac{kd}{2L}x\right) \right|.$$

8. Why does time not appear in the formula for amplitude, Equation (2)?

**Answer** Because amplitude means 'maximum displacement' we determine for each location  $x$  what the maximum value of the displacement is in time. Then the amplitude will not depend on time anymore.

9. Finally: Is it a general characteristic of a wave that there is a change in time? Do we need such a property in order to understand interference? You might want to use the expression for  $\hat{u}_{\text{pattern}}$  to answer this question.

**Answer** Generally speaking, a wave is a periodically changing phenomenon, in space as well as in time. We have used this characteristic in the above calculations. Firstly because water waves change in time. Secondly, we can see this from the expression for  $\hat{u}_{\text{pattern}}$ . If we would add two static waves, we would never get the amplitude from Equation (2), but a snap shot of the animation.

### 1.1.2 Light

A double slit experiment for light was first described by Thomas Young in 1804. On the screen, opposite to the double slit, a static pattern is now visible. A picture of this static pattern is shown in Figure 3. We compare the pattern of water with that of light (respectively Figures 2 and 3 on page 3). Note that the water pattern is shown from above, whereas the light pattern is shown on the screen opposite to the double slit.

1. How can the animation of the expression for  $\hat{u}_{\text{pattern}}$  help us to compare the two patterns with each other? Describe similarities and differences between the two patterns.

**Answer** Figure 2 is a top view of the setup from Figure 1, whereas Figure 3 shows the pattern visible on the screen, as shown in Figure 1. To compare the two domains

### 1.1.3 Electrons

A double slit experiment for electrons was first conducted by Claus Jönsson in 1961. Figure 4 on page 3 shows the pattern that is visible when electrons are sent through a double slit. Just in the case of light, this pattern is static.

1. How can we compare the pattern in Figure 4 to that of water and light (Figures 2 and 3)? You might want to use the animation for  $\hat{u}_{\text{pattern}}$ . Describe similarities and differences between the several patterns.

**Answer** Again it is striking that there are places where no electrons hit (corresponding to places where we do not see the water oscillating) and places where many electrons hit (places where the water oscillates strongly). The main difference is that we do not see the wave itself: we do not observe something going up and down, only the number of electrons.

2. Why do bands appear with many, and few electrons if we combine two “electron beams” (the electrons emerging from the two slits)? How can we understand this behavior if we think of the assignment on the double slit experiment for water? Systematically map terms from water to electrons in order to answer this question.

**Answer** We can understand this if we assume that we can describe electrons with waves, just as we did for water and light. From each of the two slits such a wave emerges and they cancel, or amplify each other.

3. Do we observe a movement in the case of electrons: something that changes in time? Do we need such a property to answer question 2?

**Answer** We do not observe a movement in case of electrons: only a static pattern. We can describe this pattern by assuming that two time dependent waves, described by Equation 1, emerge from the two slits.

4. What relation might there be between the amplitude and the observed electrons?

**Answer** The pattern we observe for electrons has the characteristics of an interference pattern, so we can postulate the existence of a wave causing this pattern. The connection between the amplitude of this wave and the observed electrons (per unit area) will be: the larger the amplitude, the more electrons, where the amplitude is zero we do not find any electrons.

(water and light) we need the expression for  $\hat{u}_{\text{pattern}}$ , which gives the displacement of the water waves along the screen. If we compare the animation with Figure 3 it is striking that we observe moving waves, whereas for light this is not be visible. What is similar is that there are places of light and dark, corresponding to places where the water is oscillating and places where the water is tranquil. What differs, is that the displacement of the water waves is visible, but of the light waves not.

2. Why do light and dark bands appear on the screen in case of two “light sources” (the two slits)? How can we understand this behavior if we think of the previous assignment on the double slit experiment for water? Systematically map terms from water to light in order to answer this question.

**Answer** The setup of both experiments maps perfectly onto each other. In both cases the two slits can be seen as two identical sources of water waves, or light beams. Comparing the patterns is somewhat difficult: the places where the water oscillates strongly (constructive interference) correspond to light places, places where the water stands still correspond to places of darkness in the case of light. Stated differently: the dark and light bands are places where the light is amplified, or canceled out. This is typical for interference. We can understand this behavior if we assume that in case of light, just as with water, waves emerge from the slits that can be described by Equation (1). The displacements of both waves add. Where they are both positive (negative), they amplify, where they are opposite, they cancel out.

3. Do we observe a movement in the case of light: something that changes in time? Do we need such a property for our answer to question 2?

**Answer** In case of light we observe a static image. We do need to assume that something is moving in time, just as was the case with water. This can explain the form of  $\hat{u}_{\text{pattern}}$  and thus the interference pattern.

4. What do we exactly observe on the screen in case of light? Is it the same as the displacement we have calculated? Give arguments pro, or con. What is qualitatively the relation between the amplitude  $A(x)$  and the brightness of the light on the screen?

**Answer** We cannot see a displacement on the screen. For two reasons: the displacement is something that can also be negative and we only see something greater than, or equal to zero. Secondly: we are seeing a static image, not something changing in time, such as the displacement.

We are thus observing something that has to do with the amplitude of the wave: the static image we could discern with some difficulty in the assignment on water. The displacement of the light waves is not observable. The qualitative relation between amplitude and light intensity (brightness): the larger the amplitude, the lighter. Where the amplitude equals zero, there is darkness (no light).

## Studio course 2: Meaning of matter waves

### 2.1 Interpretation of the wave function

⊕ In the assignment on the double slit we have had a close look at interference of water, light, and electrons. The interference pattern of electrons was made by aiming a beam of electrons on a double slit. In this assignment we closely watch how the pattern builds up. Again we have a double slit, but we now fire very few electrons: 1000 per second. The source accelerates the electrons with a voltage of  $V_0 = 50$  kV.

1. How much time is there between two consecutive electrons? What speed do the electrons have? So what would their distance be if they could move unhindered?

**Hint** the kinetic energy of the electrons is determined by the voltage  $V_0$  with which they are accelerated.

**Answer** The time between two electrons is  $\Delta t = 1/1000$  s. The speed is determined by the kinetic energy they gain by the voltage of 50 kV:  $E_{\text{kin}} = eV_0$ . Because (classically)  $E_{\text{kin}} = \frac{1}{2}mv^2$ , the speed of the electrons equals:  $v = \sqrt{\frac{2eV_0}{m}}$ . Their (average) distance is thus:

$$\Delta x = v\Delta t = \sqrt{\frac{2eV_0}{m}}\Delta t = \sqrt{\frac{2 \cdot 1.6 \cdot 10^{-19} \text{ C} \cdot 50 \text{ kV}}{9.1 \cdot 10^{-31} \text{ kg}}} \cdot 1/1000 \text{ s} = 130 \text{ km}.$$

2. Based upon the previous answer: how many electrons are there at a given time in the apparatus? Make a rough estimate of the length of the apparatus.

**Answer** We can safely assume that the experimental setup has a size in the order of one meter. At any instance there is at most one electron in the apparatus. If there would be more than one electron in the apparatus, their distance would be far less than 130 km.

A film was made of the build up of the electrons on the screen. Watch the film on Blackboard: Assignments → Studio Course 2.

3. What is so characteristic about the way in which the pattern is built up?  
**Answer** Electrons appear one by one in a seemingly random way. Only when enough electrons have hit the screen, can we discern a pattern that shows interference. The interference pattern is thus a property of many electrons. Is does not make any sense to speak of interference in the case of a few electrons.
4. What aspects of the film can we explain by the wave function we introduced in the assignment on the double slit?

**Answer** With the wave function we can understand the pattern of many electrons, not where an individual electron will hit the screen. We can thus predict the probability for an electron to hit at a particular place.

5. In the case of water we say that water waves interfere and give rise to an interference pattern. Indicate to what extent we can say this in the case of electrons.

**Answer** The electrons do not interfere with each other: they are too far apart for that. We do however see interference. The conclusion must be that the matter waves interfere.

6. In what sense does the wave function tell us something about an individual electron? What is (qualitatively) the relation between the amplitude  $A(x) = |\psi|$  and the number of electrons hitting a specific point?

**Answer** The wave function only says something about the probability for an electron to hit the screen at a particular point. The amplitude  $A(x)$  is a measure for the probability to find an electron in a small region around  $x$ .

7. Sometimes one speaks of the wave-particle duality in quantum mechanics. What can you say about this duality based on the assignments about interference?

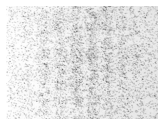
**Answer** On the one hand we observe wave-like behavior: an interference pattern is visible. On the other hand we still observe individual electrons, as particles.

### 2.2 Intermezzo: Potential energy and force (classically)

The electrons in the double slit experiment are in a special way hindered in their movement by the barrier (the double slit). In this way the surroundings determines the behavior of the electrons. We can describe the surroundings by the force that acts on the electrons at certain locations. Another way is by looking at the potential energy, or potential in short, of the electrons. In general the potential describes the interaction between a particle and its surroundings. It thus determines how the particle will behave, classically as well as quantum mechanically. In this assignment we will therefore have a closer look at the concept of potential and its relation to force.

In the following we will write  $E_{\text{kin}}$  for kinetic energy (sometimes denoted by  $T$ ) and  $V$  for potential (energy). Do not confuse the latter with electrical potential (potential energy per unit charge)!

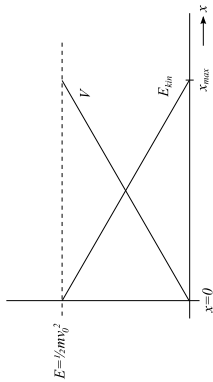
We consider a ball of mass  $m$  that is thrown upwards from the ground with an initial speed of  $v_0$ . We choose the  $x$ -axis such that it increases in the upward direction. In that case the gravitational force is negative (points downwards):  $F_g = -mg$ .





1. First sketch the graph of the kinetic energy  $E_{\text{kin}}$  and the potential (energy)  $V$  of the ball as a function of its height. Put the height  $x$  on the horizontal axis (the ground is at  $x = 0$ ) and the energy on the vertical axis. Indicate in the graph what the total energy is and how high the ball will get. You do not have to calculate anything for this!

**Answer** As the potential energy of a mass due to a gravitational force equals  $mgh$ , and the total energy  $E$  is conserved, the graph would look something like this:



2. Under certain conditions it is possible to define a potential for a force that only depends on the position of the particle, such that:

$$F(x) = -\frac{dV(x)}{dx}. \quad (3)$$

Use this formula to determine the potential that corresponds to the gravitational force.

**Remark** Note that only a *change* of potential results in a force.

**Answer** The gravitational potential energy equals  $mgh$ , or  $mgx$  with the correct variable. Substituting this into formula (3) gives:

$$F = -\frac{dmgx}{dx} = -mg.$$

3. We next consider the interaction between two electrical charges. The potential for a charge  $e$  with respect to a charge  $-e$  that are at a distance  $r$  from each other, is given by:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r},$$

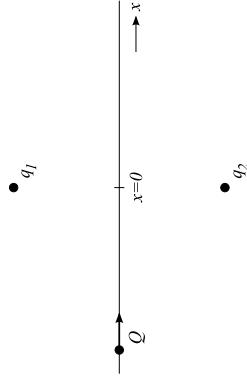
where  $\epsilon_0$  is the permittivity of vacuum and  $e$  the elementary charge. This potential is called the Coulomb potential. What force corresponds to this potential? Sketch the potential as function of  $r$ . Keep in mind that  $r \geq 0$ .

**Hint** Equation (3) holds here as well, but now the variable is  $r$  instead of  $x$ .

**Answer** The force that corresponds to this potential is obtained by filling in the expression for the potential in Equation (3):

$$\begin{aligned} F(r) &= \frac{d}{dr} \frac{e^2}{4\pi\epsilon_0 r}, \\ &= \frac{e^2}{4\pi\epsilon_0} \frac{d}{dr} \frac{1}{r}, \\ &= -\frac{e^2}{4\pi\epsilon_0 r^2}. \end{aligned}$$

4. Finally, have a look at the following figure:



The figure shows three equal positive charges  $Q$ ,  $q_1$  and  $q_2$ . The charges  $q_1$  and  $q_2$  cannot move: as though they are fixed. Charge  $Q$  can only move along the  $x$ -axis and enters from the left with a certain velocity.

- (a) What will determine whether charge  $Q$  is able to pass charges  $q_1$  and  $q_2$ ?

**Answer** The charge  $Q$  will only pass the two charges  $q_1$  and  $q_2$  if it goes fast enough. The two charges will slow down charge  $Q$ .

- (b) Sketch the force that charge  $Q$  will experience along the  $x$ -axis. Choose the force positive when it points to the right, and negative when it points to the left.

**Answer** Left of the two charges, the force will be directed to the left and becomes stronger as the distance to the two charges decreases. Somewhere in front of the two charges, the force is maximal and will be zero between the two charges. To the right of the two charges the force becomes positive (directed to the right), becomes maximal somewhere after the two charges and then diminishes. The graph will be anti-symmetric (odd) with respect to the origin (at  $x = 0$ ).

(c) Sketch the potential that charge  $Q$  “feels” along the  $x$ -axis.

**Answer** The potential equals the area under the force graph (with a minus). The graph of  $V(x)$  has the shape of a hill, with its maximum at  $x = 0$ .

(d) Suppose that at the far left charge  $Q$  does not feel any influence of charges  $q_1$  and  $q_2$ : the potential energy is zero there, and  $Q$  only has kinetic energy. What will happen to the kinetic and potential energy of the charge as it moves closer to the two fixed charges? Try to represent this in the graph of the potential you have sketched in the previous question. Under what condition will charge  $Q$  pass the two charges?

**Answer** If the charge moves closer to  $q_1$  and  $q_2$ , the kinetic energy will decrease and the potential energy will increase. The sum will remain constant: the total energy is conserved. This can be depicted in the graph with a horizontal line for the total energy. The kinetic energy is the difference between the total and the potential energy. If the total energy is larger than the maximum of the potential energy, charge  $Q$  will pass.

## Studio course 3: Probability

### 3.1 Electron diffraction by a straight edge

In the assignments on the double slit and the interpretation of the wave function we have seen that the particle density on the screen has to be an increasing function of the wave amplitude. We do not yet know the form of this function. We therefore consider an experiment where the double slit is replaced by a straight edge in the center of the electron beam (see Figure 7). Behind the double slit the number of electrons is measured at different locations along the screen.

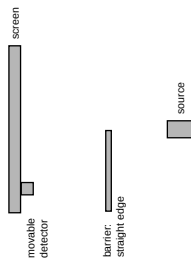


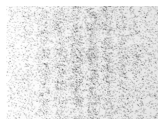
Figure 7: Setup of the experiment with the straight edge.

1. Reason how you might calculate the displacement of the wave at the detector (see Figure 7), analogues to the method in the double slit assignment. Try to express this in words.

**Answer** With the double slit the waves from the two slits add up. Now we do not have one slit, but virtually a sequence of slits next to each other, without a separation between them: each point is a slit from which a circular wave emerges. These all add up. This is Huygens principle. The displacement of the wave at a certain point along the screen is the sum of all displacements of the contributing waves.

2. How large do you expect the amplitude (maximum displacement) of the wave to be far left (behind the edge) and far right (from the edge)? Express this in term of  $A_0$ : the amplitude you would expect without the edge. What do you expect the amplitude will be precisely in the center of the setup, i.e. right behind the edge?

**Answer** With the straight edge in the setup we have half the number of sources (refer to the previous answer). If we consider the sources (along the barrier) in symmetric pairs (left and right, round the center of the setup), then for each source at a distance of  $x$  from the center axis, a source at a distance  $-x$  is missing. Because



for the point:  $x = 0$  on the screen each source in a pair is at an equal distance from the middle of the setup, the effect will be that the displacement is halved. So at  $x = 0$  the amplitude will equal  $\frac{1}{2}A_0$ . Far left no electrons will hit, the expected amplitude will be zero. Far right the effect of the edge is negligible, the amplitude there will equal  $A_0$ .

We will compare the expected amplitudes (of the presupposed wave) from question 2 to the actual measured electrons. Refer to Figure 8. The vertical axis shows the number of detected electrons  $I$  proportional to the number of electrons that would have been measured without the edge ( $I_0$ ). The horizontal axis gives the location of the detector:  $x = 0$  corresponds to the center of the setup on the screen,  $x < 0$  behind the edge and  $x > 0$  in the beam. The electrons have been measured by placing the detector at different locations along the screen (the  $x$ -axis) for a fixed time.

3. What is the number of electrons measured far left ( $x \ll 0$ ), in the middle ( $x = 0$ ) and far right ( $x \gg 0$ ) on the screen, behind the edge? Put these values in a table, together with the amplitudes from question 2.

	$x \ll 0$	$x = 0$	$x \gg 0$
$A/A_0$			
$I/I_0$			

Formulate a conclusion: what is the relation between the number of electrons and the (presupposed) amplitude? Explain how you have reached your conclusion.

**Answer:** The table will look something like this:

	$x \ll 0$	$x = 0$	$x \gg 0$
$A/A_0$	0	$\frac{1}{2}$	1
$I/I_0$	0	$\approx 0.5$	0

Right behind the edge we find approximately  $I/I_0 = 0.25$ . The relation between  $I$  and  $A$  seems to be:  $I/I_0 = (A/A_0)^2$ . In general one would expect the relation between the amplitude of the wave and the electron density to be  $I \propto A^2$ . The proportionality is due to the fact that the units of the two quantities differs; there must at least be some constant involved.

### 3.2 Classical probabilities

Because the function with which we describe the electrons has something to do with probabilities, we will next have a closer look at probabilities, averages and expectation values. For this assignment we will make use of an applet of

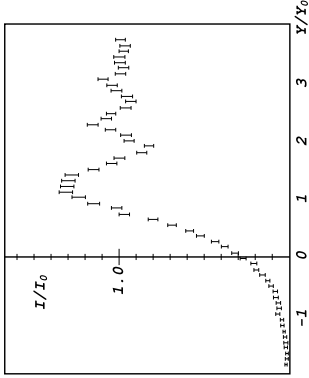


Figure 8: Number of measured electrons behind the straight edge, along the  $x$ -axis. The length of the bars indicate the inaccuracy of the measurement.

an oscillating spring. You can find this on the Blackboard site of this course: **Assignments** → **Studio Course 3** → **trillende veer**. Open the applet, and continue with the assignment.

We imagine that each 0.1 second a photo is taken of the setup. The region in which the ball moves back and forth ( $-10 < x < 10$ ) is divided in ten intervals of equal length. For each photo we take we determine in which of the ten intervals the center of the ball is located. We do this for all photo's and add up the result. This results in the table (right) with the corresponding histogram (left, below). You can start the applet by pressing **[start]**. By pressing the button **[>>]** you step through all photo's. Another useful function: click in the graph and you get the coordinates under the mouse pointer. Clicking the right mouse button opens a window with a copy of the graph at that instant.

1. Let the ball oscillate for 25 seconds and then press **[pause]**. In total we now have 250 photo's. What is the probability of finding the ball for instance round  $x = -7.37$  if we would make a photo at an arbitrary moment? Determine this probability with use of the histogram.

**Hint:** First determine in what interval  $x = -7.37$  is located and then read off in the table how often the ball has been found in that interval. Use this to calculate the probability.

**Answer:** The position  $x = -7.37$  corresponds to the second interval (from the left). After 25 seconds I have 22 photo's in that interval. In total 250 photos were made, so the probability equals  $22/250 = 0.088$ .

2. The probability you have calculated corresponds to a region *round*  $x = -7.37$  where the ball can be found. What is the precision of the location of the ball?

**Answer** The given location is in the second interval, lying between  $-8$  and  $-6$ , so the location is determined with an accuracy of  $\Delta x = 2$ .

3. We now search for a general expression for the probability of finding the ball in a certain interval. Let  $n_i$  be the number of times the ball is found in the  $i$ -th interval. Express the probability  $p_i$  of finding the ball in the  $i$ -th interval in terms of  $n_i$ . What is the total probability (i.e. to find the ball at an arbitrary location)? Check this with the general expression for the probability you have found.

**Answer** We create a general recipe based on the answer from question one:  $p_i = n_i/n_{\text{tot}}$ , with in this case  $n_{\text{tot}} = 250$ . The total probability, the sum of  $p_i$ , should be equal to 1:  $\sum_i p_i = \sum_i n_i/n_{\text{tot}} = \frac{1}{n_{\text{tot}}} \sum_i n_i = \frac{n_{\text{tot}}}{n_{\text{tot}}} = 1$ , so this is consistent.

4. What do you expect the average position of the ball is? How could you calculate this? If the ball is found in the  $i$ -th interval, we use the center of the interval for its position and call this  $x_i$ . Try to give a general expression in terms of the probability  $p_i$  (your previous answer).

**Answer** The movement of the oscillator is symmetric round  $x = 0$ , so the average position will be equal to  $x = 0$ . This can be calculated as follows. The average is the sum of the number of times the ball is found at a certain position multiplied by the position it is found, divided by the total:  $\langle x \rangle = \sum_i x_i n_i / n_{\text{tot}} = \sum_i x_i p_i$ . This is actually the expectation value!

5. How can we determine more precisely the probability the ball is found round a certain position (more than one answer possible)?

- a) By making the intervals smaller (more intervals);
- b) By making photos over a longer period of time;
- c) By making photos at a higher frequency in the same time.

Try this out with the applet and calculate for each new setting the probability of finding the ball round  $x = -7.37$ . Write down the settings you have used. Put your data in a table:

#int.	#photo's	prob.
10	250	...
10	500	...
25	250	...
⋮	⋮	⋮

**Answer** First of all we have to make the intervals smaller. This determines the precision a particular probability can be calculated (refer to answer 2). If we do not make enough photos however, the number of photos in each interval might become too small and imprecise. It is not sufficient to make more photos: errors could be introduced by a special combination of frequency of oscillation and the width of an interval. It is better to increase to frequency with which we take photos. The correct answer is a) and c). The table could look like this (with photo-frequency 10 and 20 Hz):

#int.	#photo's	prob.
10	250	22/250 = 0.088
10	500	46/250 = 0.092
25	250	9/250 = 0.036
25	500	19/500 = 0.038
50	250	9/250 = 0.018
50	500	20/500 = 0.020

6. Based on the table you have made: what do you think the probability is of finding the ball at a certain location? Is this useful to us?

**Answer** The probability goes to zero, this is not useful.

We will now try to find an expression that says something about the probability of finding the ball and at the same time is a property of a particular position.

7. Extend the above table with a column in which you write down the probability *divided* by the width of the intervals  $\Delta x$  used. For instance, when we have 10 intervals,  $\Delta x = 20/10 = 2$ . What happens to the values in this extra column with increasing number of intervals? Do you think we can use this expression?

**Answer** Extending the above table gives:

#int.	#photo's	prob.	prob./ $\Delta x$
10	250	22/250 = 0.088	0.044
10	500	46/250 = 0.092	0.046
25	250	9/250 = 0.036	0.045
25	500	19/500 = 0.038	0.048
50	250	9/250 = 0.018	0.045
50	500	20/500 = 0.020	0.050

This value remains more or less constant, and as  $\Delta x \rightarrow 0$  this says something about a particular position.

## Studio course 4: A new theory

### 4.1 An equation for $\Psi$

In the assignment on the double slit experiment for electrons we have seen that we could describe the electrons with a wave function of the form:

$$\Psi(r, t) = Ae^{i(kr - \omega t)}.$$

In the experimental setup of the double slit, the electrons move freely from both slits through the vacuum to the screen. With “freely” we mean that no forces act on the electrons. From classical physics however we know that a particle’s movement is influenced by the forces that act on it. This should be accounted for in the quantum theory we are setting up.

In this assignment we will search for an equation from which the wave function  $\Psi$  can be calculated for more general situations. To keep it simple we will look at one dimensional systems. We assume that the wave function for a *free* electron, without forces acting upon it, will look like this:

$$\Psi(x, t) = Ae^{i(kx - \omega t)}. \quad (4)$$

This is almost the same function as at the beginning of this assignment, except that  $r$  has been replaced by  $x$ . In other words: we will look at an electron that can only move along the  $x$ -axis.

To find an equation for  $\Psi$  it is wise to start from what is known to us: classical physics.

1. Why is it *not* sensible to start from Newton’s second law:

$$F = ma(t) = m \frac{d^2x(t)}{dt^2}, \quad (5)$$

where  $x(t)$  is the trajectory of the particle? Think of the meaning we have given to the wave function  $\Psi$ .

**Answer** It is not sensible to start from Newton’s second law because there we need to be able to speak of the trajectory of the particle: at any instance of time it is known where the particle is located. This is in contradiction to what we have found so far: the description of electrons by a wave entails that we do *not* know where the electron exactly is. The wave function only tells us with what probability the electron will hit at a certain location.

2. Why would it be reasonable to start from the total energy of the electron:

$$\begin{aligned} E &= E_{\text{kin}} + V, \\ &= \frac{1}{2}mv^2 + V(x), \\ &= \frac{p^2}{2m} + V(x), \end{aligned} \quad (6)$$

8. The values in the last column are called probability densities: probabilities per unit length in this case. In the previous question you have only calculated the probability density for the interval in which  $x = -7,37$  lies. We could repeat this for each interval. The probability densities for the different intervals can then again be set out in a histogram. Sketch this histogram for the case we have 10 intervals.

**Answer** The histogram equals the histogram from the applet, but then we have to multiply the  $y$  axis by a factor  $1/n_{\text{tot}}\Delta x$ .

9. Suppose we decrease the width of the intervals, and let  $\Delta x$  go to zero. We then get a *function*  $\rho(x)$  that gives the probability density for each point  $x$ . Based on the histogram from the last item, sketch the graph for  $\rho(x)$ .

**Answer** The function fluently follows the histogram.

10. How might you use the graph of  $\rho(x)$  to determine the probability of finding the ball between, for instance  $x = -2$  and  $x = 3$ ? Try to give a general expression in terms of  $\rho(x)$ .

**Hint** What would the total area under the graph of  $\rho(x)$  be?

**Answer** The probability to find the ball between  $x = -2$  and  $x = 3$  is given by the area under the graph between those two points. Mathematically:

$$P_{a-b} = \int_a^b \rho(x) dx.$$

The total area under the graph should be equal to 1.

with  $p$  the momentum of the electron, and  $V(x)$  its potential?

**Answer:** It is reasonable to start from total energy. Firstly because then it is possible to consider energy conservation, secondly because we know that waves have a certain energy.

Let us first search for an equation for  $\Psi$  of which the solution is the wave function of the free particle, Equation (4). For a free particle  $F(x) = 0$ , and  $V(x) = V_0$  (constant). We first choose  $V_0 = 0$ . For the total energy we then have:

$$E = \frac{p^2}{2m}. \quad (7)$$

3. What is the relation between the momentum  $p$  and the wave number  $k$  of an electron (de Broglie)? What is the relation between the energy  $E$  and the angular frequency  $\omega$  of an electron? Try to use these expressions to rewrite Equation (7) for the total energy with as much wave quantities instead of classical quantities.

**Remark:** Recall that  $f = \omega/2\pi$  and  $\lambda = 2\pi/k$ .

**Answer:** We have that  $p = h/\lambda = \hbar k$  and  $E = hf = \hbar\omega$  (de Broglie-Einstein relations). These expressions can be used in the equation for the total energy (with  $V = 0$ ):

$$\begin{aligned} E &= \frac{p^2}{2m}, \\ \hbar\omega &= \frac{(\hbar k)^2}{2m}, \\ &= \frac{\hbar^2 k^2}{2m}. \end{aligned}$$

4. In Newton's second law, Equation (5), the acceleration is calculated from the particle's position by taking the second derivative. In analogy to this, how could we extract the wave number  $k$  from the wave function  $\Psi(x, t)$ ? And the same for the angular frequency  $\omega$ ? Use this to rewrite the expression from the previous item such that  $\Psi$  occurs in it.

**Hint:** Start by calculating the first and second derivatives of  $\Psi(x, t)$  with respect to the time  $t$ , and the position  $x$ . Decide which derivatives you can use.

**Answer:** Following the hint:

$$\begin{aligned} \frac{\partial \Psi(x, t)}{\partial t} &= -i\omega \Psi(x, t) \\ \frac{\partial^2 \Psi(x, t)}{\partial t^2} &= -\omega^2 \Psi(x, t) \\ \frac{\partial \Psi(x, t)}{\partial x} &= ik \Psi(x, t) \\ \frac{\partial^2 \Psi(x, t)}{\partial x^2} &= -k^2 \Psi(x, t) \end{aligned}$$

The second derivative with respect to time is not useful;  $\omega^2$  does not occur in our energy equation. Likewise, there is no use for the first derivative with respect to the position. The other derivatives are used to find an expression for  $\omega$  and  $k^2$ :

$$\begin{aligned} \omega &= i \frac{\partial \Psi(x, t)}{\Psi(x, t)} \frac{\partial t}{\partial t} \\ k^2 &= - \frac{1}{\Psi(x, t)} \frac{\partial^2 \Psi(x, t)}{\partial x^2} \end{aligned}$$

If we use this in the expression for the energy, we find:

$$\frac{\hbar \frac{\partial \Psi(x, t)}{\partial t}}{\Psi(x, t)} = - \frac{\hbar^2 \frac{\partial^2 \Psi(x, t)}{\partial x^2}}{\Psi(x, t)}.$$

Dividing by  $\Psi$  looks ugly, so we multiply left and right by  $\Psi$ :

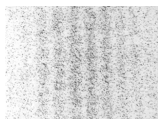
$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = - \frac{\hbar^2 \partial^2 \Psi(x, t)}{2m \partial x^2}.$$

It could be that students use the following expression for  $k^2$ :

$$k^2 = - \frac{1}{\Psi^2} \left( \frac{\partial \Psi}{\partial x} \right)^2.$$

This will fail at the point where we demand that the differential equation should be linear (questions 7 and 8). Should the student find at that later point that the equation is not linear, then he should be asked if there is another way to find an expression for  $k^2$  (i.e. the second derivative).

5. When we choose another reference point  $V_0$  for the potential, the total energy  $E$  will change such that the kinetic energy, and thus the physics will remain the same. Reason that  $E$  changes in the following manner:  $E \rightarrow E' = E + V_0$ , where  $E'$  is the new energy. Use this to rewrite the result from question 4 such that it holds for arbitrary, but constant  $V_0$ .



**Answer** The total energy changes, the kinetic energy remains the same. For the total energy we had found:

$$E' = h\omega' = \frac{i\hbar}{\Psi'(x,t)} \frac{\partial \Psi'(x,t)}{\partial t}.$$

The primes are to indicate that we have a different wave function and a different value for  $\omega$ . The kinetic energy was equal to:

$$E_{\text{kin}} = E = -\frac{\hbar^2}{2m} \frac{1}{\Psi(x,t)} \frac{\partial^2 \Psi(x,t)}{\partial x^2}.$$

Combining this to  $E' = E + V_0$ , we find:

$$\frac{i\hbar}{\Psi'(x,t)} \frac{\partial \Psi'(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\Psi'(x,t)} \frac{\partial^2 \Psi'(x,t)}{\partial x^2} + V_0.$$

It is convenient to multiply both sides with  $\Psi'$ , and dropping the prime:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V_0 \Psi(x,t).$$

6. The equation you have found up to now is a differential equation. The solution to this differential equation is our assumption for  $\Psi$  for the free particle, i.e. Equation (4). Check that Equation (4) is indeed a solution to our differential equation.

The differential equation thus does not tell us anything we did not know before we started. How could you adjust the equation so that it tells something for the case we have an arbitrary potential  $V(x)$ ? Is Equation (4) then still a solution?

**Answer** When we insert the wave function from Equation (4) in the differential equation, we can see it is a solution when the following holds:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V_0.$$

We can adjust the differential equation by substituting  $V(x)$  for  $V_0$ . Now (4) is not a solution anymore, because then it should hold that:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x),$$

but this can not be the case for all  $x$ .

7. A differential equation often has more than one solution, depending on the boundary conditions. Of linear homogeneous second order differential equations with constant coefficients we know that the sum of two solutions is also a solution.

Is it desirable that our equation has this property of addition? Give arguments based on the double slit experiment.

**Answer** In the double slit experiment we have seen that adding two waves gives rise to the interference pattern. Each of the two separate wave functions could describe an electron that emerges from one of the two slits. The addition then means that it is now no longer known through which slit the electron has traveled. The most general addition is:  $\Psi = c_1 \Psi_1 + c_2 \Psi_2$ . This should also be a solution to our differential equation.

8. Does the differential equation you have found in 6 satisfy the new property under 7? If not: try to satisfy this property without losing other desired properties.

**Answer** We assume that both  $\Psi_1$  and  $\Psi_2$  are solutions to our differential equation:

$$\begin{aligned} i\hbar \frac{\partial \Psi_1}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1}{\partial x^2} + V(x) \Psi_1, \\ i\hbar \frac{\partial \Psi_2}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2}{\partial x^2} + V(x) \Psi_2. \end{aligned}$$

Adding this gives:

$$i\hbar \left( \frac{\partial \Psi_1}{\partial t} + \frac{\partial \Psi_2}{\partial t} \right) = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi_1}{\partial x^2} + \frac{\partial^2 \Psi_2}{\partial x^2} \right) + V(x) (\Psi_1 + \Psi_2)$$

Then the sum  $\Psi = \Psi_1 + \Psi_2$  should also be a solution (for simplicity we choose  $c_1 = c_2 = 1$ ):

$$i\hbar \left( \frac{\partial \Psi_1}{\partial t} + \frac{\partial \Psi_2}{\partial t} \right) = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi_1}{\partial x^2} + \frac{\partial^2 \Psi_2}{\partial x^2} \right) + V(x) (\Psi_1 + \Psi_2).$$

This equals the previous result. (We have used the linearity of the differential operators  $\partial/\partial x$  and  $\partial/\partial t$ .)

If all went according to plan you have found a differential equation for  $\Psi(x,t)$ . We started from a small number of assumptions for  $\Psi(x,t)$  and an equation from classical physics we have trusted upon, i.e. the expression for the total energy. We will have a last critical look at this result:

9. Explain whether we have given a *derivation* of the equation for  $\Psi$  with the above? Would you expect that a derivation is possible? Give arguments.

**Answer** This is not a derivation. It is not to be expected that we can give one, because classical physics falls short. This means we have to add something to it. This is a creative process. Of course we want to preserve certain things from classical physics. That is why we started from the expression for the total energy.

10. At the beginning of this assignment we used a complex function for  $\Psi$ . In the double slit experiment for water we used such a form for the first time to describe our wave. We there were only interested in the real part of the complex wave. Using complex numbers was a “trick” to simplify the calculations (although you might not have experienced it like that). What is the status of using a complex wave in our new, own made differential equation?

Check whether the real part of our wave function, Equation (4), could satisfy the differential equation. What is your conclusion? Is something wrong with the equation, or is something wrong with using a real wave function?

**Answer** When we try as possible solution:  $\Psi(x, t) = A \cos(kx - \omega t)$ , we get:

$$i\hbar A \sin(kx - \omega t) = \frac{\hbar^2 k^2}{2m} A \cos(kx - \omega t) + V(x) A \cos(kx - \omega t).$$

This can never be a solution for all  $x$  and  $t$ ; on the left is a sine, on the right a cosine. It is not to be expected that the differential equation for  $\Psi$  is wrong. It has all desired properties. The complex wave function also correctly describes the interference pattern. It seems that the wave has to be complex. This is not a problem. The wave function itself has not been given a physical meaning. We can use it to calculate a probability density (which is real) and make a connection with experimental outcomes. Of course, when starting out with a real wave, the derivatives we have calculated would also be different. However, to express  $\omega$  and  $k$  in terms of these derivatives would require us to take a square root somewhere. We would then lose the required property of linearity.

Because we cannot be sure our equation is correct, we do the following. We assume it to be correct: it is a postulate. We will have to see how this will work out. If the predictions we make based on this equation are correct, we get more faith in its validity. The differential equation is called the Schrödinger equation, named after Erwin Schrödinger who first wrote it down in 1926.

#### 4.2 Information in the wave function: operators

In the following we will define the wave function  $\Psi(x, t)$  as a solution to the Schrödinger equation. In classical physics we often try to find a function  $x(t)$ ; the location of a particle at a certain moment in time. As soon as we have found this function, we can determine other physical quantities from it, like for instance the velocity  $v(t)$ , the acceleration  $a(t)$  and the momentum  $p(t)$ . We have already concluded that a function  $x(t)$ , actually the trajectory of a particle, is not to be expected in quantum mechanics. In this assignment we will see whether we can find expressions for physical quantities, like for instance the momentum, in quantum mechanics.

1. To arrive at the Schrödinger equation we have used the de Broglie relation  $p = \hbar/\lambda = \hbar k$ . This relation relates a momentum to a certain wavelength. Explain how we can determine the momentum directly from  $\Psi(x, t)$ . Review the steps taken in the previous assignment.

**Answer** In the previous assignment we have already found a way to do this. We found  $k$  by taking the first derivative with respect to position and then had to multiply with  $-\hbar$ . Because  $p = \hbar k$ , we get the following:

$$\hat{p} = -\hbar \frac{\partial}{\partial x}.$$

2. How could we, similarly, find the kinetic energy from  $\Psi(x, t)$ ? Compare this result to the Schrödinger equation. Comment on this.

**Hint** Classically, the kinetic energy is given by:  $E_{\text{kin}} = \frac{1}{2} m v^2 = \frac{p^2}{2m}$ .

**Answer** The kinetic energy is classically given by  $E_{\text{kin}} = p^2/2m$ . For  $p$  we can use our quantum mechanical version. What does the square of a derivative mean? The square of the derivative does not make sense to me: we can try to see it as a second derivative. So taking the first derivative twice.

$$\hat{E}_{\text{kin}} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

This term occurs exactly in the Schrödinger equation. This is not strange: we have found this equation by using an expression for the kinetic energy.

In the assignment where we have found an equation for  $\Psi$ , we have seen that the sum of two solutions is itself again a solution. Thus, if  $\Psi_1$  and  $\Psi_2$  are solutions, then  $\Psi = \Psi_1 + \Psi_2$  is a solution as well. What about the momentum of such a solution? Suppose we have the following solutions:

$$\begin{aligned} \Psi_1(x, t) &= A e^{i(kx - \omega t)}, \\ \Psi_2(x, t) &= A e^{i(-kx - \omega t)}. \end{aligned}$$

3. Read off what the momentum is of  $\Psi_1$  and what the momentum is of  $\Psi_2$ . **Answer** The first wave function has a wave number  $k$ , and thus a momentum  $p_1 = \hbar k$  (using de Broglie). Similarly, the second wave function has a momentum  $p_2 = -\hbar k$ . We might also use our expression for  $p$  for  $\Psi_1$  and  $\Psi_2$ . We then get:

$$\begin{aligned} \hat{p}\Psi_1 &= \hbar k \Psi_1, \\ \hat{p}\Psi_2 &= -\hbar k \Psi_2. \end{aligned}$$

The momentum of  $\Psi_1$  probably is  $\hbar k$ , and that of  $\Psi_2$  probably  $-\hbar k$ . The first describes a particle going to the right (for instance) and the other a particle going to the left.



4. Give an expression for the sum  $\Psi = \Psi_1 + \Psi_2$ . What would you think that the momentum is now, based on the momentum of  $\Psi_1$  and  $\Psi_2$  separately? Try to use your method from question 1 to determine the momentum.

**Answer** The sum of  $\Psi = \Psi_1 + \Psi_2$  is given by:  $\Psi = A e^{i(kx - \omega t)} + A e^{i(-kx - \omega t)} = 2A \cos(kx) e^{-i\omega t}$ . I do not know what the momentum is. After all, the first wave function describes something going to the left, the other something going to the right. If we try to determine the momentum, we get:

$$\hat{p}\Psi = -i\hbar k 2A \sin(kx) e^{-i\omega t}.$$

I cannot make sense of this.

5. Think back to the assignment on the double slit experiment. There we called the sum of two wave functions (states) a *superposition*. How did we interpret such a superposition? What was the relation between such a superposition and conducting a measurement? Again answer the previous question: what is the momentum of the superposition  $\Psi = \Psi_1 + \Psi_2$ ?

**Answer** We have interpreted a superposition as describing two possible measurement outcomes: we either measure the particle going to the left, or we measure a particle going to the right. The momentum is thus not clearly defined.

6. To prevent confusion with the classical momentum  $p$ , we denote the quantum mechanical momentum as  $\hat{p}$  and call it the momentum operator. Describe differences and similarities between  $p$  and  $\hat{p}$ .

**Answer**  $p$  is a number,  $\hat{p}$  not; it does something to a function. We therefore call it an operator. You get a number back if you let  $\hat{p}$  operate on (particular) wave functions. If this is a wave function with a clearly defined momentum, then the result of  $\hat{p}$  is the same as what you would expect of  $p$ : the momentum. For more complicated wave functions it does not make sense to speak of the momentum.

### 4.3 Expectation values

We now have a (differential) equation for the wave function  $\Psi$  and an idea how to extract information from the wave function. However, there is something strange: a superposition does not always have a specific momentum. How can that be? If we think of the wave function as describing the probability of finding the particle in certain region, then it is not strange to expect that for the momentum something similar holds. It is to be expected that  $\Psi$  also expresses the probability of finding the particle with a certain momentum. In this assignment we will further investigate this idea.

1. In assignment 3.2 we talked about probabilities. How did we calculate the probability of finding the particle in a certain region? How did we calculate the expectation value  $\langle x \rangle$  of the location. All classically!

**Answer** If the probability density is given by  $\rho(x)$ , then the probability of finding the particle in the interval  $[a, b]$  is given by:  $P_{a,b} = \int_a^b \rho(x) dx$ . The expectation value then is calculated as follows:  $\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x) dx$ .

2. How do you think we can calculate the quantum mechanical expectation value  $\langle x \rangle$  of the location  $x$ ?

**Answer** The probability of finding the particle in the interval  $[a, b]$  is now given by:  $P_{a,b} = \int_a^b \Psi^* \Psi dx$ . The expectation value is calculated as follows:  $\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi dx$ .

3. In the previous assignment we found an operator with which we could determine the momentum of wave function:

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}.$$

How could you calculate the expectation value  $\langle p \rangle$  of the momentum, using this operator?

**Answer** We try:  $\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi dx$ . We can look at this as follows: the operator  $\hat{p}$  gives the momentum of the wave function times the wave function. Next,  $\Psi^* \Psi$  gives the probability density.

4. Suppose we have some kind of operator  $\hat{O}$ . How can you determine the expectation value  $\langle O \rangle$  of this operator?

**Answer** Analogous to the expression for  $\hat{p}$  we would get:  $\langle O \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{O} \Psi dx$ .